

STATISTICAL THEORIES OF SOLID SOLUTION HARDENING

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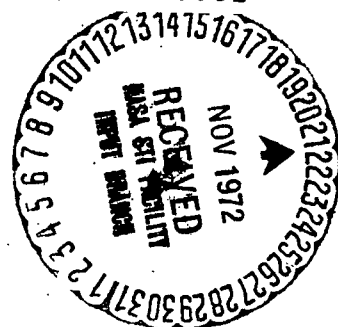
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# STATISTICAL THEORIES OF SOLID SOLUTION HARDENING

R. Labusch<sup>1</sup>

ABSTRACT: Theoretical approaches to the problem of solid solution hardening are critically analyzed and some modifications and extensions to existing theories are suggested. The significant parameters of solid solution hardening are the concentration  $c$  of solute atoms, the range of interaction  $w$  between solute atoms and dislocations, the strength  $f_0$  of the interaction and the line tension  $T$  of the dislocation. All theories, if carried out correctly, yield either  $\tau_c \sim c^{2/3} f_0^{1/2} T^{1/3} w^{1/3}$  or  $\tau_c \sim c^{1/2} f_0^{2/3} T^{1/2}$  for the relation between these parameters and the critical shear stress  $\tau_c$ . Usually the first of these relations holds under the conditions found in experiments while the other one is valid only if  $cw^2 < 10^{-3}$ , i.e., in the limit of extremely small  $w$  or small concentrations.

## 1. Problem Definition

Let us assume that the motion of dislocations is hindered by a statistical /917\* distribution of foreign atoms (FA) or other obstacles, the interaction of which (W.W.) is assumed to be known. The W.W. of a single obstacle may be described by an internal stress field

$$\sigma_H = \sigma_0 \cdot \phi_1\left(\frac{x}{v}, \frac{w}{y}\right) \quad (1)$$

where  $x, y$  are coordinates in the slip plane parallel and perpendicular to the dislocation. (In general, internal stresses will be designated by  $\sigma$  and the externally applied shear stress by  $\tau$ ). More complex W.W. with more than two characteristic lengths are naturally possible, but in order to avoid unnecessary complications, the present work will be restricted to the simplest case. In place of Eq. (1), another statement may be chosen

$$\sigma_H b = \frac{f_0}{v} \phi\left(\frac{x}{v}, \frac{y}{w}\right) \quad (2)$$

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\* Numbers in the margin indicate pagination in the foreign text.

Here the obstacle is described by the force it exerts on the dislocation. Let  $f_0$  be the total interaction force acting on the straight dislocation. It is typical for solid solution hardening (MKH) that this force is weak, i.e., that the angle  $\theta_1$ , by which the direction of the dislocation is altered through interaction with an obstacle is small compared to 1:  $\theta = f_0/T \ll 1$ , where  $T$  is the linear stress.

The density of obstacles will be given, depending on the context in which it is used, as volume concentration  $c_v$ , atomic concentration  $c_{at}$ , or surface concentration  $c$  in the slip plane. The three values are readily converted into each other. If the obstacles consist of single F.A., then  $c_v = c_{at}/\Omega = c/h$ , where  $\Omega$  is the atomic volume and  $h$  the distance between adjacent lattice planes.

The problem for which a solution is to be found, consists of the calculation of the shear stress  $\tau_c$ , which causes a dislocation to migrate over arbitrary distances. Let us also assume that the free movements of the dislocations is sufficiently damped (by phonons and electrons) so that dynamic effects are negligible and that the movement is sufficiently slow on the average so that an instantaneous equilibrium is established at all times. The start of the motion of the dislocations is designated the critical state and  $\tau_c$ , the critical shear stress. The problem is complicated by the fact that the line stress prevents individual line elements of the dislocation from occupying positions of minimum free energy independently of each other, and therefore cannot be solved by the conventional methods of statistics. For this reason, it is capable of adapting itself to the statistical field of the obstacles to a certain degree only and this adaptation degree in turn depends on the number and strength of the obstacles: fewer strong obstacles force better adaptation than a greater number of weak obstacles.

## 2. Dimensional Analysis

The first publication in which this fact was recognized and considered are those by Mott and Nabarro [1-3]. Prior to embarking on an analysis of these and more recent attempts to solve the problem, it appears suitable to conduct a dimensional investigation to determine in a very general manner the type of results that can be expected in principle from a statistical theory; if only a single type of obstacles exists in the slip plane, the dislocation in static

equilibrium can be described by the following equation:

$$T \frac{\partial^2 y}{\partial x^2} - \frac{f_0}{v} \sum_v \phi \left( \frac{x - x_v}{v}, \frac{y - y_v}{w} \right) + \tau b = \sigma \quad (3)$$

The shape of the dislocation line is a solution of this equation with periodic boundary conditions, where the length of period is assumed to be equal to the macroscopic dimensions of the crystal are to the mesh width of the dislocation network. The mathematical signs are chosen so that positive values of  $f_0 b/v$  correspond to a W.W. force acting in the negative  $y$  direction. In accordance with the assumptions, the start of the motion of dislocations may be considered a sequence of static equilibria. Therefore, the form of the dislocations must represent a solution of Eq. (3) even in the critical state. Five parameters appear in this equation:  $T$ ,  $f_0$ ,  $v$ ,  $w$ , and  $c$ ; the concentration  $c$  is implicitly included in the  $(x_v, y_v)$  distances of the obstacles. Introduction of the dimensionless variables  $\xi = x \sqrt{c}$  and  $\eta = y \sqrt{c}$  yields a system in which distances are independent of  $c$ . Following division of the equation by  $T$ :

$$\frac{\partial^2 \eta}{\partial \xi^2} - \frac{f_0}{v \sqrt{c} T} \sum_v \phi \left( \frac{\xi - \xi_v}{v \sqrt{c}}, \frac{\eta - \eta_v}{w \sqrt{c}} \right) + \frac{\tau b}{T \sqrt{c}} = 0 \quad (4)$$

Any variation of  $c$  thus is transformed into variations of the characteristic lengths  $v$  and  $w$ . This eliminates one of the five original parameters. The exact solution for  $\tau_c b$  may contain only the parameters  $f_0/v \cdot \sqrt{c}$ ,  $T$ ,  $v \sqrt{c}$ ,  $w \sqrt{c}$  and  $\tau_c b/T \sqrt{c}$ . Exactly

$$\tau_c b = T \sqrt{c} \Psi \left( \frac{f_0}{v \sqrt{c} T}, v \sqrt{c}, w \sqrt{c} \right) \quad (5)$$

where  $\Psi$  is a function to be determined by the theory. Usually, the result is a product of the powers of the parameters involved. The result then may be written as follows:

$$\tau_c b = \text{const.} \cdot f_0 \cdot \left( \frac{f_0}{T} \right)^\alpha c^{(1-\beta)/2} w^\beta \left( \frac{v}{w} \right)^\gamma \quad (6)$$

Since  $v/w$  is a dimensionless number of the order of magnitude of one, the theory in essence must yield a coefficient and the exponents  $\alpha$  and  $\beta$ . It must also be expected that  $\alpha > 0$ , because  $\tau_c$  must certainly be a declining function of  $T$ . (For  $T \rightarrow \infty$ , the dislocation is always a straight line. Fitting to the statistical obstacle field is then impossible and the average of all W.W. forces

on the dislocation is zero, with the exception of statistical variations which decline in magnitude per unit length with increasing length of the dislocation).

This general consideration is of interest for the evaluation of detailed theories: the result of a theory must not contradict Eq. (6). It is also interesting that in some cases in contradiction to the condition of  $\alpha > 0$ ,  $\tau_c \sim f_0$  is found experimentally, i.e., for body-centered cubic metals. It must then be concluded that the fundamental Eq. (3) is not applicable, which is actually expected due to the role played by the Peierl potential in the metals. Finally, it may be concluded from Eq. (5) that for point obstacles, i.e., in the boundary case of  $v\sqrt{c} \rightarrow 0$ ,  $w\sqrt{c} \rightarrow 0$ ,  $\tau_c b \sim \sqrt{c}$  must be true exactly; since the boundary value of  $\tau_c$  cannot be neither zero nor infinite,  $\Psi$  must be such that  $\lim \Psi = \Psi_0(f_0/T)$ . Then

$$\lim_{\substack{v\sqrt{c} \rightarrow 0 \\ w\sqrt{c} \rightarrow 0}} \tau_c b = T \cdot \sqrt{c} \cdot \Psi_0\left(\frac{f_0}{T}\right) \quad (7)$$

where it is also required that  $\Psi_0(f_0/T)$  be more than proportional to  $f_0 T$ , so that  $\tau_c b$  may become a declining function of  $T$ . In actual fact, both detailed theories [4-6] and computer experiments [7] always yield  $\tau_c \sim \sqrt{c}$  for point obstacles. /919

### 3. The Statistical Theories of Mott and Nabarro and of Asimov and others

In order to better compare the different approaches and solutions, let us select a representation somewhat different from the original theories, while utilizing their fundamental ideas and arguments.

Mott and Nabarro begin with a statistical internal stress field with a characteristic wavelength  $\lambda$  and a typical amplitude of  $\sigma_a \cdot \lambda$  which is set equal to  $c_v^{-1/3}$ , which must be further discussed. Since  $\theta \ll 1$  (see Chapter 1), the dislocation cannot adapt itself to this stress field. The linear average of  $\sigma$  thus always acts on a length of  $L \gg \lambda$ . The statistical variations of the linear averages are taken as the effective obstacles. The average amplitude of the oscillations, designated by  $\sigma_L$  is a function of  $L$ .  $L$  is then selected so that complete adaptation to the effective obstacles is possible. For this purpose, it is necessary that the effective stress field with an amplitude  $\sigma_L$  impose a

wave character with an average wavelength of  $L$  and an amplitude of  $\lambda$  on the dislocation (Figure 1).

Then, it must be true that

$$\frac{1}{2} \left( \frac{L}{2} \right)^2 \frac{\sigma_L b}{T} \approx \frac{\lambda}{2} \quad (8)$$

due to the assumed perfect fit

$$\tau_c \approx \sigma_L \quad (9)$$

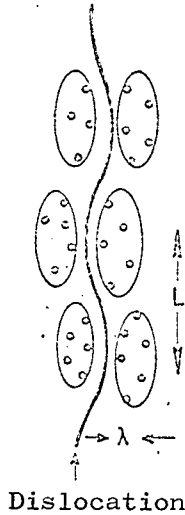


Figure 1. Effective obstacles in the theory by Mott and Nabarro.

Mott and Nabarro then argue that in accordance with the rules of statistics the oscillations of the average of  $\sigma$  over  $L$  are equal to the amplitude  $\sigma_a$  divided by the root of the number of wavelengths  $\lambda$  which fit into  $L$ :  $\sigma_L = \sigma_a \sqrt{\lambda/L}$ . They use the linear average of the stress  $|\sigma_H|$  of a single obstacle over a volume of  $V_c = 1/c_v$  for the amplitude  $\sigma_a$ . This yields

$$\sigma_L = \sqrt{\frac{\lambda}{L}} \cdot \frac{1}{V_c} \int_{V_c} |\sigma_H| d^3r \quad (10)$$

Mott and Nabarro set  $\lambda = c_v^{-1/3}$ . Elimination of  $L$  from the Eqs. (8) and (10) yields:

$$\tau_c \sim \sigma_0^{4/3} c_{at}^{11/9} T^{-1/3} \log c_{at} \quad (11)$$

Here, it is assumed that the stress field of an individual obstacle declines for large distances  $r$  with  $1/r^3$ .

The concentration dependence implied in Eq. (11) has not been observed experimentally. If, however, one makes an effort to modify the theory in its weak points, experimentally well confirmed results are obtained; the weakness of the theory of Mott and Nabarro lies in their calculation of  $\sigma_L$  and their assumption concerning the value of  $\lambda$ . Let us first discuss  $\sigma_L$ . The decisive point here appears to be the linear averaging of  $\sigma_H$  in the calculation of the amplitude  $\sigma_a$ . Actually,  $\sigma_a$  is not even needed, because the correct formula for  $\sigma_L$  according to the methods of statistics is  $\sigma_L = E(\langle \sigma \rangle_L^2)$ , where  $E(\langle \sigma \rangle_L^2)$  is the expected value of the square of  $\langle \sigma \rangle_L$  and the  $\langle \sigma \rangle_L$  the average of  $\sigma$  over the

length  $L$ . In the calculation of the expected value one must consider that foreign atoms are fixed on lattice planes which may assume  $z$  coordinates, i.e., discrete values. In contrast, the dislocation line may assume arbitrary positions in the slip plane, so that  $x$  and  $y$  pass through a continuum. Then

$$E(\langle \sigma \rangle_L^2) = \frac{h}{V} \sum_n \iint_{-\infty}^{+\infty} dx dy \left\{ \int_x^{x+L} \sigma(x', y, (n + \frac{1}{2})h) dx' \right\}^2 \quad (12)$$

where  $h$  is the distance of lattice planes parallel to the slip plane and  $V$  a large standard volume.

It is seen here that lattice planes adjacent to the slip plane furnish an overwhelming contribution to the MKH. If  $\sigma_H$  declines with  $1/r^3$ , the  $n^{\text{th}}$  term of  $\angle 920$  the sum in Eq. (12) is proportional to  $1/(n + \frac{1}{2})^4$ , i.e., the contribution of the two adjacent planes twice removed is to the contribution of the two immediately adjacent planes as 1 is to 81.

If  $L \gg v$ , then

$$E = c/L \cdot \sum_n \iint_{-\infty}^{+\infty} \left[ \int_{-\infty}^{+\infty} \sigma_H(x', y, (n + \frac{1}{2})h) dx' \right]^2 dx dy$$

This yields  $E \sim (c/L) f_0^2 (w/b)$  and

$$\sigma_L = A \cdot \frac{f_0}{b} \sqrt{\frac{cw}{L}} \quad (13)$$

The numerical factor  $A$  is a function of the exact form of W.W. It is of the order of magnitude of 1.  $f_0$  has been defined in Eq. (2).

The assumption of  $\lambda \approx c_v^{-1/3}$  again does not stand up to an accurate statistical analysis. Statistics yield [8, 9]

$$\lambda = \pi \sqrt{\frac{S}{S_1}} \text{ with } S = E(\langle \sigma \rangle_L^2) \text{ and } S_1 = E\left(\left\langle \frac{\partial \sigma}{\partial y} \right\rangle_L^2\right)$$

$\lambda$  is also proportional to the correlation length of the statistical stress field. A precondition of the validity of this relationship is that numerous single obstacles contribute to  $\sigma_L$ , this, however, has been assumed in any case.

Evaluation of  $E\langle\langle\partial\sigma/\partial y\rangle\rangle_L^2$  with the methods used for  $E\langle\langle\sigma\rangle\rangle_L^2$  then yields

$$\lambda = \pi B \cdot w \quad (14)$$

where B is again a numerical factor of the order of magnitude of 1.

Substitution of Eq. (14) in Eq. (8) and the solution of Eqs. (8) and (13) with respect to  $\sigma_L$  results, with consideration of Eq. (9) in

$$\tau_c b = A' \cdot f_0^{1/3} c^{2/3} w^{1/3} T^{-1/3} \quad (15)$$

$A'$  is again of the order of magnitude of 1.

This relationship is in agreement with the exception of the coefficient with the result of a much more detailed statistical theory, which will be discussed later. It has been confirmed by a great number of experimental measurements.

The method used by Riddhagni and Asimov [10] closely resembles our modification of the theory of Mott and Nabarro. In place of  $\sigma_L$ , here the oscillation square of the W.W. energy  $\epsilon$  is calculated, which, however, is fundamentally the same.  $L$  is determined by minimizing the total energy, composed of linear energy and the W.W. energy

$$\frac{\partial}{\partial L} \left( \frac{T\Lambda^2}{L} + \sqrt{E\langle\epsilon\rangle_L^2} \right) = 0 \quad (16)$$

where  $\Lambda$  characterizes the amplitude of the wave character of the dislocation. This yields a relationship between  $L$  and  $\Lambda$  analogous to Eq. (8). The relationships between  $\tau_c$  and  $\sigma_L$  is obtained as follows: if  $\Lambda$  is taken as a free parameter, then  $\tau_c = \chi(\Lambda) \cdot \sigma_L$ , where  $\chi(\Lambda)$  is a dimensionless correlation function with a half value width of  $\lambda$ , which for  $\Lambda \ll \lambda$  is proportional to  $\Lambda$  and for  $\Lambda \gg \lambda$  tends asymptotically toward 1. (For details of the argument see the original paper). It now appears convenient to maximize  $\tau_c$  with respect to  $\Lambda$ . Instead,  $\Lambda$  is set arbitrarily equal to an atomic distance in the slip plane.  $\chi^{(\Lambda)}$  is assumed to be proportional to  $\Lambda$ . This procedure is questionable, because as seen previously,  $\lambda \approx w$  and  $w$  in turn depends on the order of magnitude of an atomic distance, so that  $\Lambda \ll \lambda$  is not true.

In the result, however, this differing procedure leads merely to a coefficient different from that in Eq. (15) and to a different power of  $w$ , while the other parameters ( $f_0$ ,  $T$ , and  $c$ ) have the same powers.

#### 4. The Fleischer Friedel Theory and the Calculation of the MKG with the Aid of a Distribution Function

The theories described in the foregoing do not represent the actual process of the fitting of a dislocation line to the statistical field of an obstacle. Qualitatively, the process may be described as follows: if an external shear stress is applied to the crystal, the dislocation initially remains at locations where  $\sigma$  is strongly positive (i.e., in opposition to motion). The dislocation bends between these positions. Through the bending, the dislocation leaves locations with negative  $\sigma$  and positions with positive  $\sigma$  occupied. In order to obtain a positive average of  $\sigma$ , complete adaptation to the positive maxima of  $\sigma$  is not necessary. The adaptation increases gradually until the line begins to tear away from the initially contacted maxima; at this time the critical state has been attained. Let us discuss in the following two theories which explicitly treat the problem of adaptation.



Figure 2. Dislocation in the critical state with point obstacles.

Fleischer and Friedel's theory [4, 5] <sup>/92</sup>

which will be discussed first, may be applied strictly to point obstacles only. In Figure 2 the way in which a dislocation fits itself to the obstacles is demonstrated. Since the range of the W.W. can be assumed to be arbitrarily small ( $w\sqrt{c} \ll 1$ ), one may distinguish between contacted and not contacted obstacles. Let the average distance between obstacles contacted be  $a$ . In the critical state  $\tau b \approx f_0/a$ . The calculation of  $a$  in the critical state is based on the following reasoning: if the

dislocation is torn from an obstacle because the maximum W.W. force has been exceeded, it passes over the surface area  $F$  and occupies the position indicated by the broken line. This increases the force acting on the rest of the obstacles so that they also become overloaded and are torn off. The tear propagates (this is called the "zipper effect"). It can be arrested only if the dislocation is captured by other obstacles during its passage over the  $F$  surface. The condition of the critical state in which the tearing process just begins is thus  $F \approx 1/c$ .

The line stress formula yields  $F = a^3 \tau b / 2T$ . Substitution of  $F = 1/c$ , solution with respect to  $L$  and substitution of the value of  $a$  obtained in this manner in the equation  $\tau_c b = f_0 / a$  yields

$$\tau_c b = f_0^{3/2} c^{1/2} (2T)^{-1/2} \quad (18)$$

In place of the consideration presented above, the applied stress may be increased beginning with  $\tau = 0$  and then it may be asked, how the average distance between the initially contacted obstacles decreases with increasing values of  $\tau$ . This takes place because the dislocation bends between the original obstacles and thus touches new obstacles. A simple derivation by Friedel [11] yields the equation  $a = \sqrt[3]{T / \tau b c}$ , which with the exception of a numerical factor has been confirmed by the exact theory [12]. If this is substituted in  $\tau_c b = f_0 / a$ , Eq. (18) is again obtained, with the exception of a coefficient. Comparison with Eq. (6) shows that the result satisfies the conditions of the general theory. The prediction that for point obstacles  $\tau_c \sim c^{1/2}$  has also been confirmed.

Even for point obstacles the theory described above is not exact, because from the beginning averages of the W.W. forces at the individual obstacles and of the distances between obstacles contacted, are used in the calculations. In an exact theory, distribution functions must be calculated for the distances and forces. However, no substantial change in the result as compared with Eq. (18) would be expected. Another coefficient would result, but the powers of  $f_0$ ,  $c$ , and  $T$  remain unchanged. The manner of executing such an exact theory is presented in the appendix.

The most important objection is directed against the assumption of point obstacles. In order to justify this assumption, it would be necessary that the range  $w$  of the W.W. should be less than the average bend  $\bar{y}_0$  between two obstacles. Otherwise, the sharp distinction between contacted and not contacted obstacles would be meaningless, and secondly, obstacles would have to be considered which occupy positions in which they do not counteract applied shear stresses but reinforce their action. Elementary algebra then yields  $\bar{y}_0 = f_0^2 / 12T \cdot \tau_c b$ . This, however, for typical values of  $f_0$ ,  $T$ , and  $\tau_c$  is practically always of the order of magnitude of  $w$  or greater, so that the most important condition of the theory is not satisfied.

## 5. Description of MKH by a Distribution Function

For an adequate description of the situation created when the range of W.W. is greater than the average bend between two obstacles, it is necessary to introduce a distribution function for the distances between the dislocation and the individual obstacles. Let us therefore define the number of obstacles per unit length by  $\rho(y) \cdot dy$ , the distance of which to the dislocation is between  $y$  and  $y + dy$ . It is seen immediately that for vanishing values of W.W.  $\rho(y)$  must be constant and equal to the area concentration  $c$ , because in this case no correlation exists between the position of the dislocation and the locations of the obstacles. Therefore,  $\rho(\pm\infty) = c$  is also true. If  $\rho(y)$  is known, the applied shear strength in a static equilibrium is obtained by simple integration /922

$$\tau b = \int_{-\infty}^{+\infty} \rho(y) f(y) dy \quad (19)$$

where

$$f(y) = \frac{f_0}{v} \int_{-\infty}^{+\infty} \phi\left(\frac{x}{v}, \frac{y}{w}\right) dx.$$

$\phi(x/v, y/w)$  is the function  $\phi$  defined in Eq. (2). In the anticipation of the integration over  $x$  and the following description of the problem with a single  $y$  coordinate, an approximation is hidden which could also be interpreted as the substitution of a Dirac- $\delta$ -function of  $x$  for the W.W. function  $\phi(x/v, y/w)$ :

$$\frac{f_0}{v} \phi\left(\frac{x}{v}, \frac{y}{w}\right) \rightarrow f_0 \phi\left(\frac{y}{w}\right) \cdot \delta(x) = f(y) \cdot \delta(x).$$

This assumption is justified if the change  $\Delta y$  in the vertical distance between the dislocation and obstacle on the length  $v$  is small compared with  $w$ . Here,  $\Delta y < v\theta/2$  is also true, with  $\theta$  the angle assumed to be small. This angle expresses the total change in direction at the obstacle and since in general  $v$  and  $w$  are of the same order of magnitude, the approximation is in fact always good.

The detailed calculation of  $\rho(y)$  is found in the original papers [13, 14], therefore only a simplified derivation is presented here.

Let us consider the average change  $\delta\bar{y}$  in the distance between the dislocation and an obstacle during a change in the average location of the dislocation by  $\delta l$ .  $\delta\bar{y}$  is the average over different configurations of all other obstacles with the exception of the one under consideration. Then

$$\delta\bar{y} = \delta l - f'(y)\delta\bar{y}(0)G(x) \quad (20)$$

$G(x)$  is the average response function with which the dislocations react to the change in the W.W. force  $f' \cdot \delta\bar{y}(0)$ . From the detailed theory

$$G(x) = \frac{1}{2\sqrt{\alpha T}} e^{-|x|/L} \quad (21)$$

where

$$L = \sqrt{\frac{T}{\alpha}} \quad (22)$$

and  $\alpha$  is equal to the average value of  $f'(y)\delta(x)$  over the entire length of the dislocation.  $\alpha$  must therefore be self-consistently determinable from  $\rho(y)$ :

$$\alpha = \int_{-\infty}^{+\infty} \rho(y)f'(y) dy \quad (23)$$

Due to the fact that  $G$  is dependent on  $\alpha$ , the effect of all other obstacles must be contained in the response function.

The description by Eqs. (20), (21), and (23) represents an approximation and is valid in this form only if the influence of the obstacles over which averaging takes place, is sufficiently blurred. In the appendix, this condition is mathematically formulated and it is shown that in the boundary case of sharply localized obstacles Eqs. (20) and (21) continue to be valid, but with

$$\alpha_1 = 3\varepsilon \int \frac{\rho(y)f'(y)}{G(0)f'(y)} dy \quad (24)$$

$3\varepsilon$  is of the order of magnitude of 1. The significance of  $\varepsilon$  is explained in the appendix. As the result, both point-like and extended obstacles may be treated with the same formalism.

It follows from Eq. (20)

$$g(y) = \frac{\partial\bar{y}}{\partial l} = \frac{1}{1 + G(0)f'(y)}$$

From this,  $\rho$  is found by the equation

$$\frac{\partial \rho}{\partial l} = - \frac{\partial}{\partial y} \left( \frac{\rho(y)}{1 + G(0)f'(y)} \right) \quad (25)$$

The derivation of this equation is found in [13]. In the critical state  $\rho(y)$  must become stationary, i.e.,  $\partial \rho / \partial l = 0$ . With the boundary condition of  $\rho(\pm\infty) = c$  the stationary distribution function becomes

$$\rho = \begin{cases} c(1 + G(0)f'(y)) & \text{or} \\ 0 & \end{cases} \quad (26)$$

The case of  $\rho = 0$  is highly important. It occurs with certainty if  $(1 + G(0)f'(y)) < 0$  because  $\rho$  cannot be negative. In this case a gap occurs in the distribution function, one edge of which may be freely chosen within certain limits while the other is determined by the preservation of the number of particles. The following must be valid:  $\int_{-\infty}^{+\infty} (\rho - c) dy = 0$ . In Figure 3 these conditions are represented for a typical W.W. function.  $1 + Gf'(y)$  is plotted against  $y$ . The left edge of the gap may be between  $y_1$  and  $y_2$ , while the corresponding right edge assumes values between  $y_1'$  and  $y_2'$ .

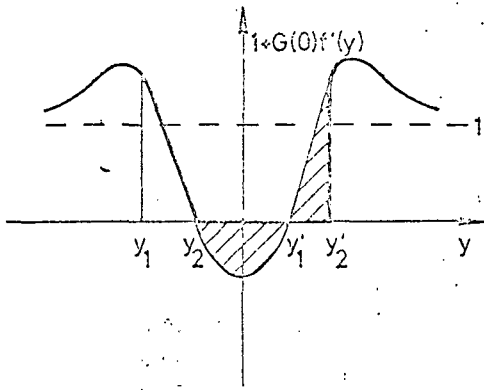


Figure 3.  $1 + G(0)f'(y)$  as a function of the distance of the dislocation to an obstacle. The left edge of the gap in the distribution function  $\rho(y)$  may be between  $y_1$  and  $y_2$ . The heavy line represents  $\rho(y)$  in the critical state for a dislocation passing to the right. Due to the preservation of the number of particles, the shaded areas must be equal to each other.

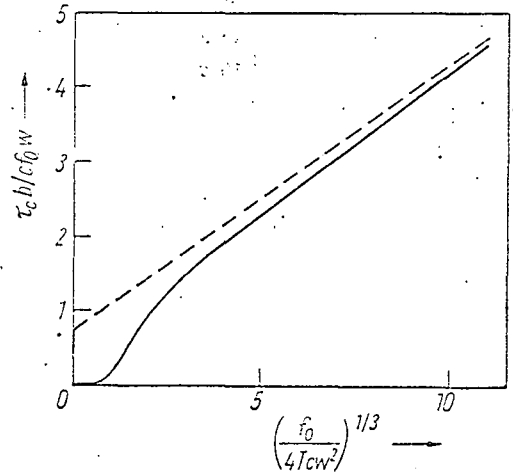


Figure 4. Theoretical dependence of the critical shear strength on the dimensionless parameter  $P = \left( \frac{f_0}{4 T c w^2} \right)^{1/3}$

(Figure 1 in (14)).

The actual position of the gap depends on the applied shear stress, because the force equilibrium requires  $\tau b = \int \rho(y) f(y) dy$  and the value of the integral is

a function of the position of the gap. If the gap is symmetrical with respect to 0, then  $\int \rho f dy = 0$ . The symmetrical position thus belongs to  $\tau = 0$ . The maximum value of  $\tau$  is attained when the left edge of the gap is at  $y_2$ . Then, the critical state is attained because the dislocations can run over arbitrary distances without further increases in the value of  $\tau$ . The system of Eqs. (19), (21), (23), and (26) must be solved numerically. Combination of the parameters in a suitable manner into dimensionless numbers yields  $\tau_c b / f_0 w c$  as a function of  $P = (f_0 / 4 T w^2 c)^{1/3}$ . This function is plotted in Figure 4.

The following was assumed for the profile of W.W.  $f(y) = f_0 (2y/w) / (1 + (y/w)^2)^2$ . It is seen that the function becomes linear for large values of the parameter  $P$ . Therefore, in this case

$$\tau_c b = \text{const.} \cdot c^{2/3} f_0^{1/3} w^{1/3} T^{-1/3} \quad (27)$$

The constant depends on the exact form of the  $f(y)$  function. Thus, the same result as with the modified Mott and Nabarro theory is obtained. If in the case of sharply localized W.W. for  $\alpha$  in place of Eq. (23), Eq. (24) is used, the following is obtained in place of Eq. (27)

$$\tau_c b \sim c^{1/2} f_0^{3/2} T^{-1/2} \quad (28)$$

The sharp decline of  $\tau_c b$  for small values of  $P = (f_0 / 4 T c w^2)^{1/3}$  in Figure 4 and the complete disappearance of the MKH at  $P \approx 1/2$  is the result of the disappearance of the distribution function  $\rho(y)$  when the maximum value of  $f'(y)$  becomes so small that everywhere  $1 + G(0)f'(y) > 0$ . This result is consistent and correct if, as has been done in the present case, a single obstacle is considered in the derivation of  $\rho$  and the other obstacles in the vicinity included through a statistical average only. It is, however, not realistic, because favorably situated groups of closely adjacent obstacles may act as a single obstacle so that in the execution of the group statistics a gap will still result in the corresponding distribution function for groups and thus a finite  $\tau_c$ . The calculation of the MKH with consideration of groups of obstacles can be performed by the following scheme: as in the theory of Mott and Nabarro, the statistical variation of W.W. averaged over a length  $L_0$  are considered effective obstacles.  $L_0$  must be of the order of magnitude of the characteristic length  $L$  of the response function as defined in Eq. (22). This yields in place of a single type of obstacles a spectrum can again be replaced by a uniform type of obstacle. The strength of these effective obstacles is  $f_{\text{eff}} = \sigma_{L_0} b L_0$ .

Substituting Eq. (13) for  $\sigma_{L_0}$  yields

$$f_{eff} \approx f_0 \sqrt{L_0 w c}. \quad (29)$$

Their number per unit area is

$$c_{eff} \approx \frac{1}{w L_0} \quad (30)$$

The width of effective obstacles is again of the order of magnitude of  $w$ . /924  
The parameter  $P$  now has the value of  $(f_0/4Tw^2c)^{1/3} \cdot \sqrt{cwL_0}$ , and is thus larger than for single obstacles. Eq. (27) thus again appears to be justified, even when  $(f_0/4Tw^2c)^{1/3}$  is not large with respect to 1. Here, however, independently of the choice of the length  $L_0$  one obtains exactly the same result as before, because  $f_{eff}^{4/3} \cdot c_{eff}^{2/3} = f_0^{4/3} c^{3/2}$ . It appears that the power law given in Eq. (27) has a more general validity than indicated by its derivation. Only in the case of point-like obstacles must a transition to the formula given in Eq. (28) be provided. In a more accurate calculation, in which a spectrum of effective obstacles is considered, it may be shown that even without application of the boundary case  $(f_0/4Tw^2c)^{1/3} \cdot \sqrt{cwL_0} \gg 1$  generally a result of the form of Eq. (27) is obtained [15]. In the extension of the theory, it must be considered that potentially the fluctuations of W.W. no longer represent weak obstacles and that their width in the direction is much greater than in the  $y$  direction so that all of the steps in the theory must be examined whether assumptions made with respect to these properties have been violated and what effect this has on the result. The fluctuation theory must certainly be applied when  $(f_0/4Tw^2c)^{1/3}$  is approximately equal to 1 or smaller. Here, this does not lead to new results, in the context of other problem definitions, such as, for example, the problem of thermal activation, differences in the statistics of single obstacles may appear.

## 6. Conclusions

The theories of the MKH may be divided into two groups. In one group, the W.W. of the dislocation with single obstacles is considered the elementary process, while in the other group, the statistical fluctuations of the W.W. averaged over a certain length, are taken as the effective obstacles. A connection between the two groups may be established in the context of a theory which describes the problem with the aid of a distribution function. The fluctuation theories yield for the critical shear stress a power law in the form of Eq. (27),

while calculation with individual obstacles leads to Eq. (27) or (28), depending on the choice of parameters. With the MKH of face-centered cubic metals, i.e., in the case of W. W. with single foreign atoms, the values of the parameters  $f_0$ ,  $c$ ,  $T$  usually are in a range in which the conditions for Eq. (28) are not satisfied. In Chapter 3, the relationship  $f_0^2/12\tau_c bT > w$  was established for this case. Substitution of Eq. (28) for  $\tau_c b$ , leads to  $(2f_0/144cT)^{1/2} > w$ . With the typical values of  $f_0/T \lesssim 10^{-1}$  and  $c \approx c_{at}/w^2$ , the condition  $c_{at} < 10^{-3}$  is obtained, i.e., the requirement of very low concentrations, where reliable experimental determination of  $\tau_c$  is usually not possible. The description by a distribution function with single obstacles requires almost the same condition:  $(f_0/4cT)^{1/3} > w^{2/3}$ , which results in the condition of  $c < 1/40$ , at the same ratio  $f_0/T \approx 10^{-1}$ . Although this condition can be satisfied in principle, it is often violated. It must thus be assumed that the MKH are normally described by a fluctuation theory with Eq. (27) as the result. On the other hand, in the case of hardening with small precipitations, to which the theories are also applicable in principle, the case of a localized W. W. is frequently realized, because here, due to the much stronger W.W. the  $f_0/T$  ratio is higher and an appreciable hardening effect occurs even with very low concentrations.

None of the theories described here considers the overcoming of the obstacles with the aid of thermal activation. The pertinent literature contains only qualitative estimates in connection with this problem. The applicability of the results is thus in a strict sense restricted to  $0^\circ\text{K}$ . Measurements, on the other hand, of MKH are usually performed at very high temperatures (for reasons of experimental convenience), on the so-called plateau range, in which the critical shear stress is independent of temperature, while it increases strongly at lower temperatures with respect to the plateau. (At low temperatures the experiments are rendered difficult by the strongly inhomogeneous slip and the occurrence of Luders bands). This process may be justified phenomenologically by the statement that  $\tau_c$  as a function of temperature behaves similarly for different values of the parameters  $f_0$ ,  $c$ ,  $T$ , and  $w$ , so that measurements in the plateau range may be taken as representative for the MKH without thermal activation. However, this similarity has not been explained satisfactorily from a theoretical standpoint and an interpretation of the existence of a plateau in place of a monotonous decline of the critical shear stress with rising temperatures is also

lacking at this time. A solution of this problem requires the incorporation of thermal activation in the statistical theory, in which the spectrum of effective obstacles, as found in the fluctuation theory, must also be considered. Suitable approaches to an extension of the theory in this sense have been presented. They lead to highly complex differential equations, which have not yet been completely solved. Preliminary calculations indicate, however, that the extended theory does in fact show the existence of a plateau and that the height of the latter is proportional to the critical shear stress calculated by neglecting thermal activation. The factor of proportionality depends only on the average velocity imparted to the dislocation by the conduct of the experiment. The extent to which a uniform dislocation velocity can be assigned to the beginning of the macroscopic plastic deformation, which defines  $\tau_c$ , must be determined. Measurements of shear stress as a function of velocity (or vice versa) at single dislocations, appear to be needed for a complete clarification of the problem.

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#### Appendix

1. Derivations of the response function used in Chapter 3 for blurred W.W. are found in [14, 15]. This formal approach cannot be applied to sharply localized obstacles. By way of a simplified model computation, first a quantitative criterion is established to distinguish between the two cases: the statistical distribution is replaced by a chain of obstacles at the same distance  $y_a$  from the dislocation and at the same distance  $a$  from each other. The response function is examined at an additional obstacle, at  $x = x_0$ . Due to the periodicity assumed,  $x_0$  can be restricted to the interval  $0 < x_0 \leq a$ . The origin of  $y$  is placed so that the additional obstacle is located at  $y = 0$ . As explained in the text, the W.W. may be treated in the  $x$  direction as Dirac-Delta-functions. Then, the dislocation is described by a differential equation of the form of Eq. (3). An increase in the applied shear stress by  $\delta\tau$  yields for the change  $\delta y$  in the position of the dislocation (see Figure 5a):

$$T \frac{\partial^2(\delta y)}{\partial x^2} - \sum_n \delta(x - na) f'(y(na)) \cdot \delta y(na) - \delta(x - x_0) f'(y(x_0)) \cdot \delta y(x_0) + \delta\tau b = 0 \quad (\text{A.1})$$

with  $f' = f'(y_a)$ .

If no additional obstacle exists, that is  $f'(y(x_0)) = 0$ , the solution of this equation consists of parabolic curves. In the interval of  $na < x \leq a(n+1)$  Figure 5 b is valid

$$\delta y_0 = \delta \tau b \left\{ \frac{a}{f'} + \frac{1}{2T} \left[ \frac{a^2}{4} - (x - a(n + \frac{1}{2}))^2 \right] \right\} \quad (\text{A.2})$$

The solution for  $f'(y(x_0)) \neq 0$  is given in the form of a sum  $\delta y = \delta y_0 + \delta y_1$ . Then  $\delta y_1$  consists of straight line segments with breaks at the locations of  $x = na$  and at  $x = x_0$  (Figure 5b). The initial statement of  $\delta y_1(na) \sim e^{\pm na/L}$  yields a solution with the condition  $2T \cdot (\cosh a/L - 1) = f' \cdot a$ . With the analogous application of the definition given in the main text in Eq. (22) of  $\alpha$ , in this case  $\alpha = f'/a$ . Then

$$2 \left( \cosh \frac{a}{L} - 1 \right) = a^2 \cdot \frac{\alpha}{T} \quad (\text{A.3})$$

It is seen that  $L$  is in agreement with the definition given by Eqs. (22) and (23) if  $(a^2 \cdot \alpha/T)$  is less than 1. A power expansion of this parameter yields

$$L = \sqrt{\frac{T}{\alpha}} \left( 1 + \frac{1}{12} a \sqrt{\frac{\alpha}{T}} \dots \right)$$

To obtain the value of the response function at  $x_0$ , the following approach is used

$$\delta y_1 = \begin{cases} A \cdot e^{-an/L} & \text{für } n \geq 1 \\ B \cdot e^{+an/L} & \text{für } n \leq 0 \\ B \cdot \left( \frac{e^{a/L} - 1}{a} x + 1 \right) & \text{in the interval } x_0 < x < a \\ A \cdot \left( \frac{e^{-a/L} - 1}{a} x + 1 \right) & \text{in the interval } 0 < x < x_0 \end{cases}$$

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It follows from the continuity at  $x_0$  that

$$\begin{aligned} \delta y_1(x_0) &= A \left( \frac{e^{-a/L} - 1}{a} x + 1 \right) \\ &= B \left( \frac{e^{+a/L} - 1}{a} x + 1 \right) \end{aligned} \quad (\text{A.4})$$

Substitution in Eq. (A.1) and integration over a small interval around the break

at  $x_0$  yields the second condition

$$\left[ -A \cdot \frac{e^{-a/L} - 1}{a} + B \cdot \frac{e^{a/L} - 1}{a} \right] \cdot T = (\delta y_0(x_0) + \delta y_1(x_0)) \cdot f'(y(x_0)) \quad (\text{A.5})$$

Elimination of A and B from Eqs. (A.4) and (A.5) leads to

$$\delta y(x_0) = \frac{\delta y_0(x_0)}{1 + \frac{a^2 + 2x_0(a - x_0)(\cosh a/L - 1)}{T \cdot 2a \sinh(a/L)} \cdot f'(y(x_0))} \quad (\text{A.6})$$

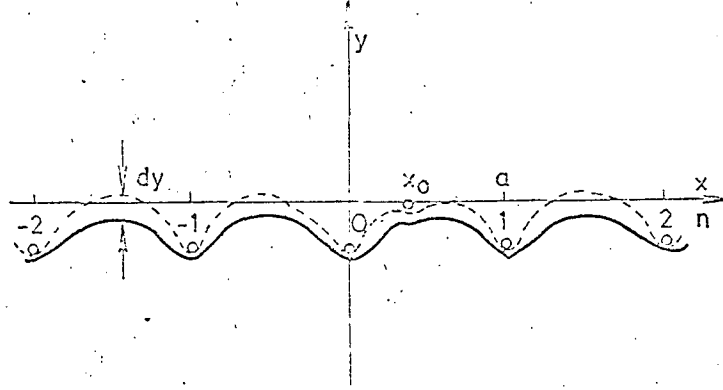


Figure 5a. A dislocation in interaction with a chain of obstacles and an additional obstacle at  $x = x_0$ . Upon increasing the applied shear strength  $\tau$  by  $\delta\tau$  the solid line changes into the broken line. The difference is  $\delta y$ .

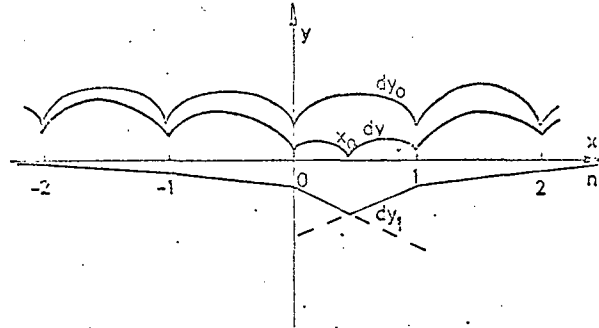


Figure 5b. The change  $\delta y$  in the position of the dislocation if the applied shear strength is increased  $\delta y$  may be divided into  $\delta y_0$  in the absence of an additional obstacle and into  $\delta y_1$  caused by the additional obstacle at  $x = x_0$ .

In this model, averaging over different  $x_0$  between zero and  $a$ :

$\bar{\delta y} = 1/a \int_0^a \delta y(x_0) dx_0$ , corresponds to averaging over different configurations.

In performing this computation, it should be noted that the average of  $\delta y_0$  is equal to the  $\delta l$  defined in the text. Power expansion of  $a/L$  shows that in the approximation in which  $L$  is in agreement with the characteristic length of the response function defined in the main text for blurred W.W., the relationship

$\bar{\delta y} = \delta l / (1 + G(0)f'(y))$  with  $G(0) = 1/2 \sqrt{aT}$  is also correct. The transition

between blurred and "localized" interactions is thus at  $a/L = 1$ , where  $L$  is to be calculated for blurred W.W. Statistical theory offers the following formula for the calculation of  $a$ :

$$a = \int_{-W}^{+W} \rho(y) dy \text{ an.}$$

2. In order to calculate the response function for localized interactions, let us return to the realistic case of the distribution of the distance between the obstacles. Let the average distance be  $\langle a \rangle$ . Let us consider again a single obstacle at a distance  $y$  from the dislocation and let us increase  $\tau$  by  $\delta\tau$ . If  $f' \langle a \rangle / T \gg 1$ , then  $\delta\bar{y}$  is small at the location of the obstacle with respect to the average displacement  $\delta l$  of the entire dislocation. Because of the force equilibrium,  $\delta\bar{y} \approx \langle a \rangle \delta\tau \cdot b/f'(y)$ . Eq. (A.2) yields, with consideration of  $\angle 927$   
 $T/f' \langle a \rangle \ll 1$  the relationship

$$\delta l = \frac{1}{a} \int_0^a \delta y_0 dx = \frac{a^2 \delta\tau b}{12T}.$$

The distribution of the  $a$  distances therefore is

$$\delta l = \frac{\langle a^2 \rangle \delta\tau b}{12T}. \quad (\text{A.7})$$

Accordingly,  $\delta\bar{y} = \delta l \cdot 12T \langle a \rangle / f'(y) \langle a^2 \rangle$ . In this case, it is stated that the obstacle has been contacted. If, however,  $\langle a \rangle f'(y)/T \ll 1$ , the obstacle is not contacted and the average displacement at the obstacle is the same as the average shift of the entire dislocation:  $\delta\bar{y} = \delta l$ . The following interpolation formula includes both cases.

$$\delta\bar{y} = \frac{\delta l}{1 + f'(y)G(0)}$$

with  $G(0) = \langle a^2 \rangle / 12T a$ . This equation is exact in the case of infinitely sharply localized interactions. The following is thus again valid:

$$\frac{\partial \rho}{\partial l} = - \frac{\partial}{\partial y} \left( \frac{\rho}{1 + f'(y)G(0)} \right).$$

It remains to express  $\langle a^2 \rangle$  and  $\langle a \rangle$  by the distribution function. We note that

$$\begin{aligned}
\frac{\partial \tau b}{\partial l} &= \int \frac{\partial \rho}{\partial l} \cdot f(y) dy \\
&= - \int f(y) \frac{\partial}{\partial y} \left( \frac{\rho}{1 + f'(y)G(0)} \right) dy \\
&= \int \frac{\rho(y)f'(y)}{1 + G(0)f'(y)} dy
\end{aligned}$$

and that on the other hand, in accordance with Eq. (A.7)  $\partial \tau b / \partial l = 12T / \langle a^2 \rangle$ .

It follows that

$$\langle a^2 \rangle = \frac{12T}{\int \frac{f'(y) \cdot \rho(y)}{1 + G(0)f'(y)} dy}.$$

Let us assume that  $\langle a \rangle^2$  is equal to  $\langle a^2 \rangle$  with the exception of a numerical factor  $\mathfrak{E}$ ; then  $G(0) = 1/2 \sqrt{\alpha_1 T}$  with

$$\alpha_1 = 3\mathfrak{E} \int \frac{f'(y)}{1 + G(0)f'(y)} dy. \quad (\text{A.8})$$

The computation of  $\mathfrak{E}$ , which is readily possible with the aid of the distribution function given in [12], has not yet been performed.

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